Contamination sources

POINT SOURCES

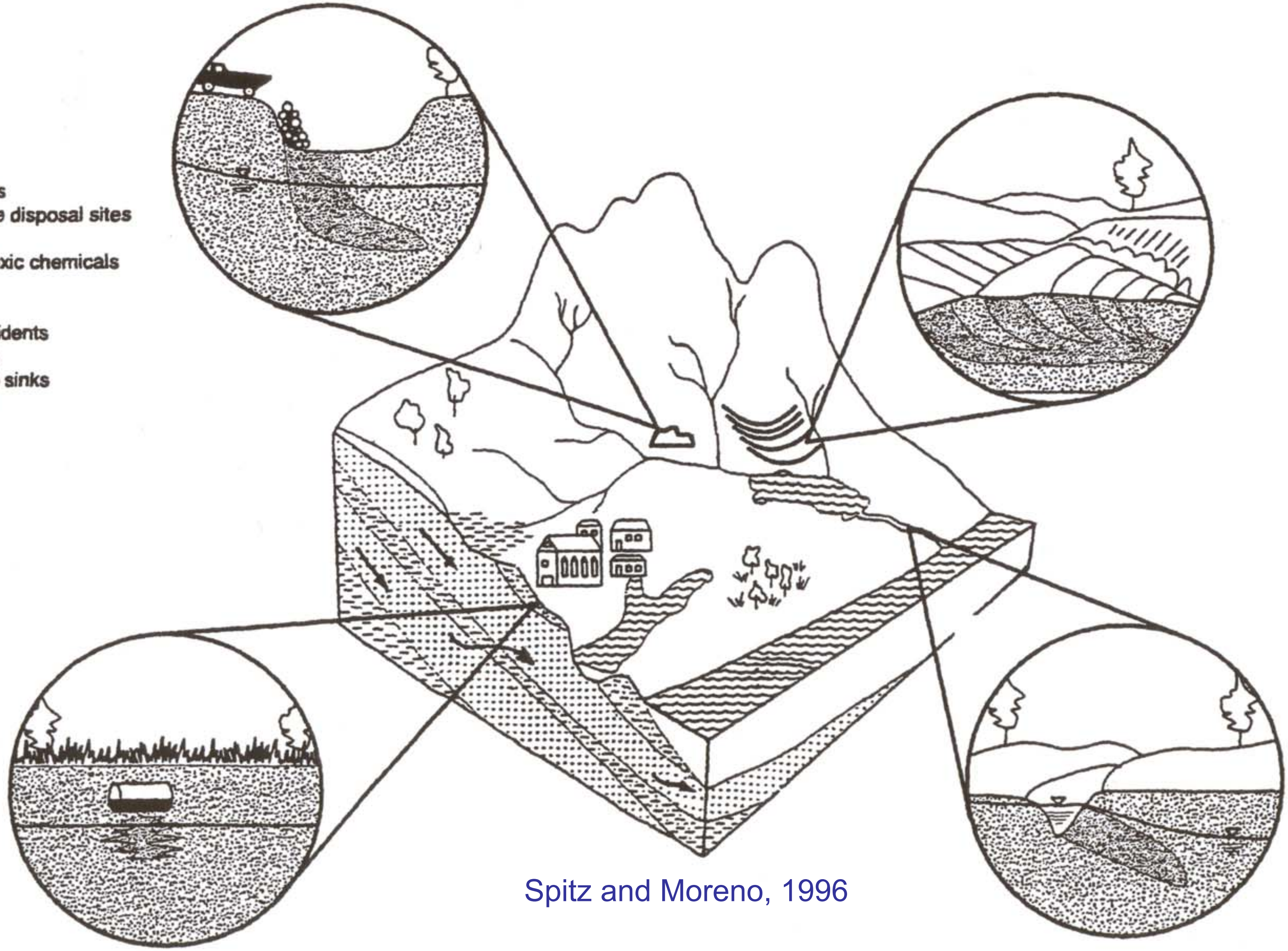
- underground storage facilities
- landfills and hazardous waste disposal sites
- surface impoundments
- illegal disposal of waste or toxic chemicals
- industrial areas
- septic tanks
- transportation spills and accidents
- injection wells and boreholes
- urban storm-water runoff into sinks
- unplugged oil and gas wells

LINE SOURCES

- underground pipelines
- sewage canals
- surface water (rivers)
- roads
- railway track

AREAL SOURCES

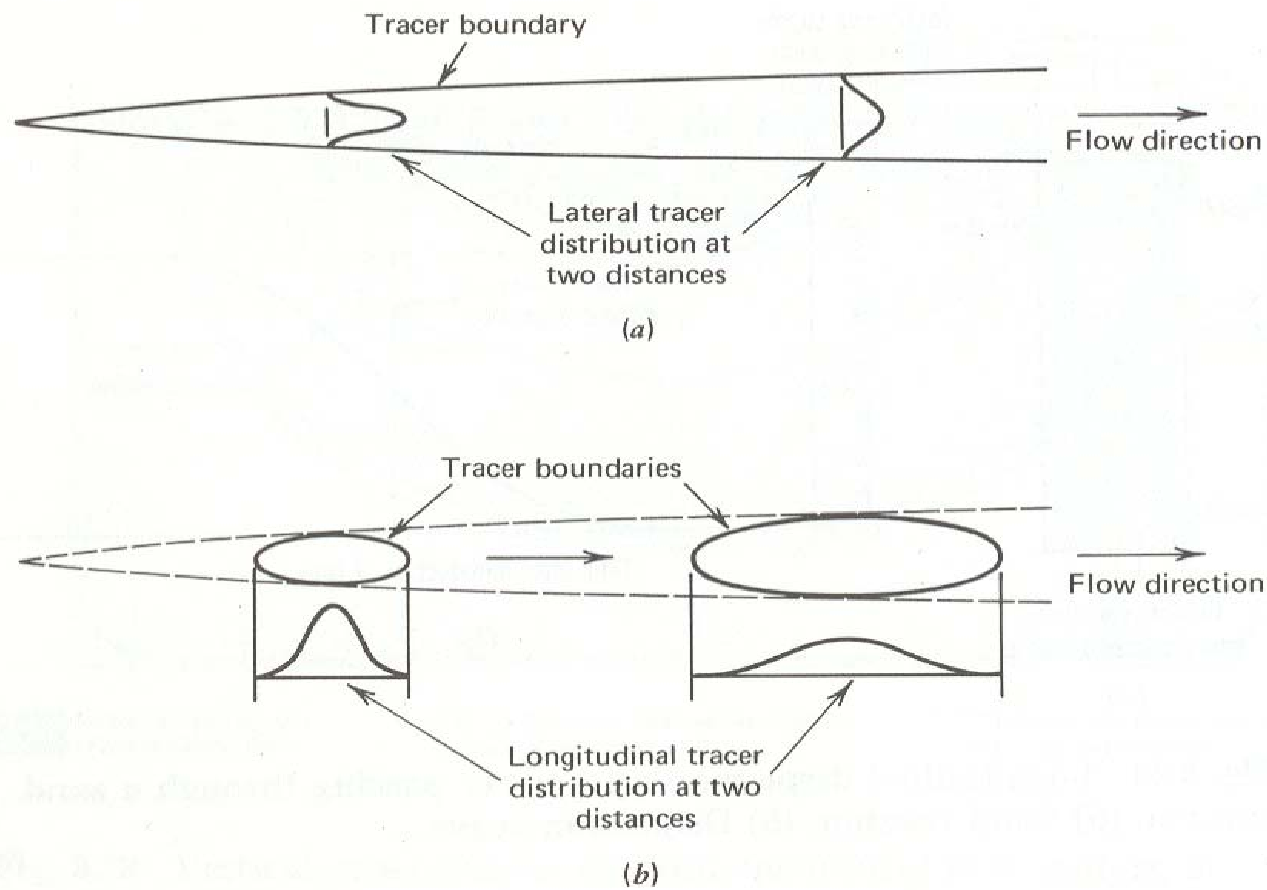
- urban areas
- industrial areas
- agricultural areas
- mining waste sites
- atmospheric components



Spitz and Moreno, 1996

Why does contaminants spread

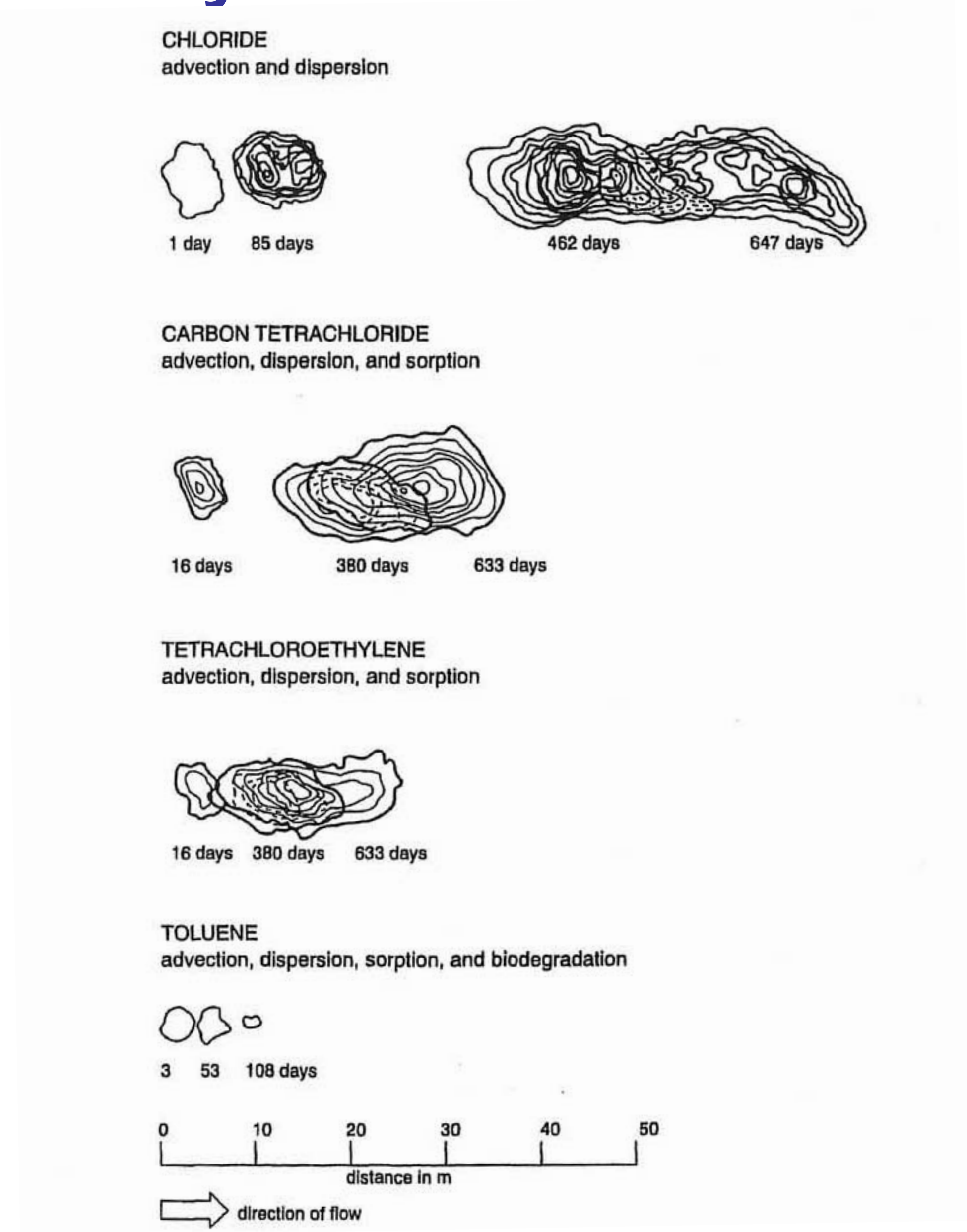
Point injection of a tracer



Spreading processes

- Advection
- Dispersion
- Diffusion
- Sorption
- Chemical reactions
- Diffusion between mobile and immobile water

Why does contaminants spread



Advection

$$\mathrm{v_a} = \frac{q}{n_e} = \frac{q}{\theta_{eff}} = -\frac{K}{\theta_{eff}}\frac{dh}{dl}$$

v_a = pore water velocity [L/T]

q = Darcy flux [L/T]

K = hydraulic conductivity [L/T]

n_e, θ_{eff} = effective porosity [-]

dh/dl = hydraulic gradient [L/L]

Advective flux

$$\mathrm{q_a} = qC = v_a C \theta_{eff}$$

C = solute concentration [M^3/L^3]

Diffusion flux

Flux of solutes from a zone with higher concentrations to a zone of lower concentrations ➔Ficks first law

$$q_0 = -D_0 \frac{\partial c}{\partial x}$$

D_0 = diffusion coefficient L^2T^{-1}

C = Solute concentration ML^{-3}

q_0 = diffusive flux MT^{-1}

Mechanical dispersion

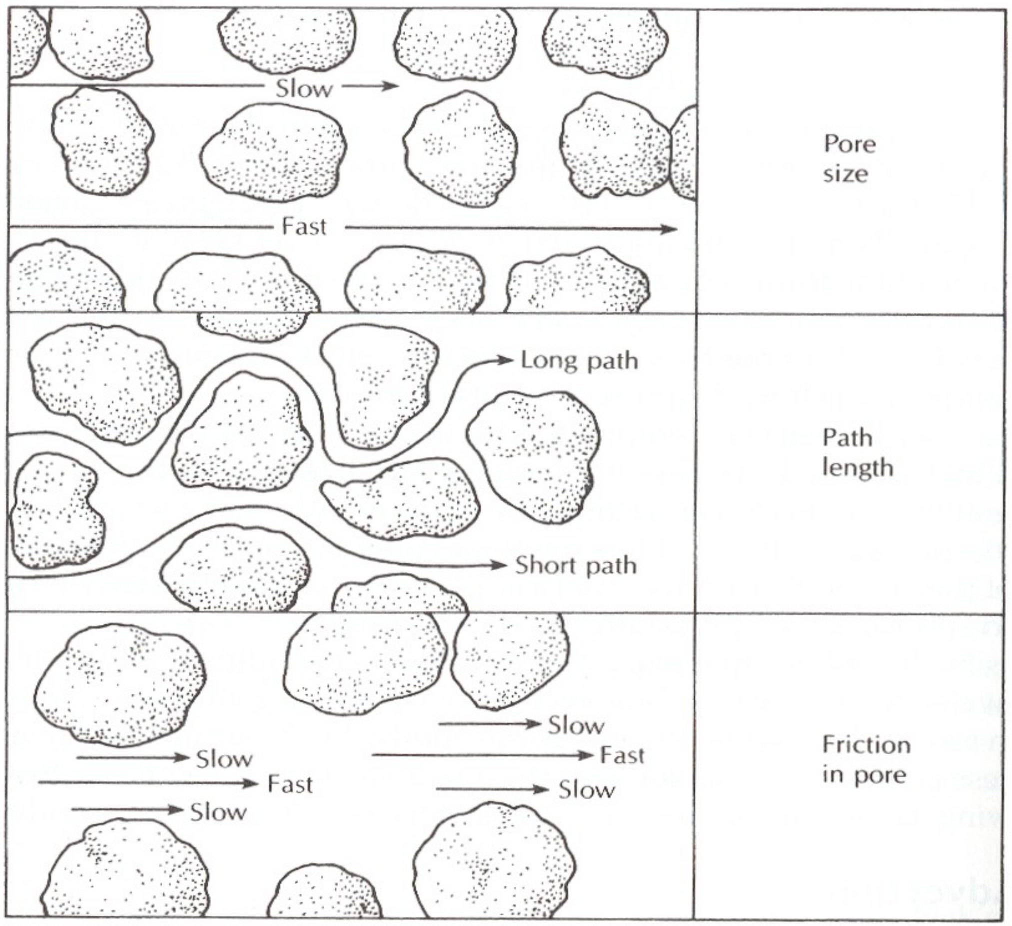
- Spreading due to pore to pore variations of the velocity field
- Spreading due to variations in the velocity field within the pores.
- Spreading due to incomplete knowledge regarding geological heterogeneities, source strength, source location, locale flow pattern, etc.

General assumption

$$\mathrm{q}_{\mathrm{M}} = -D_M \frac{dC}{dx}$$

Variations in the flow field – point scale

Longitudinal dispersion



Longitudinal dispersion
(1D flow)

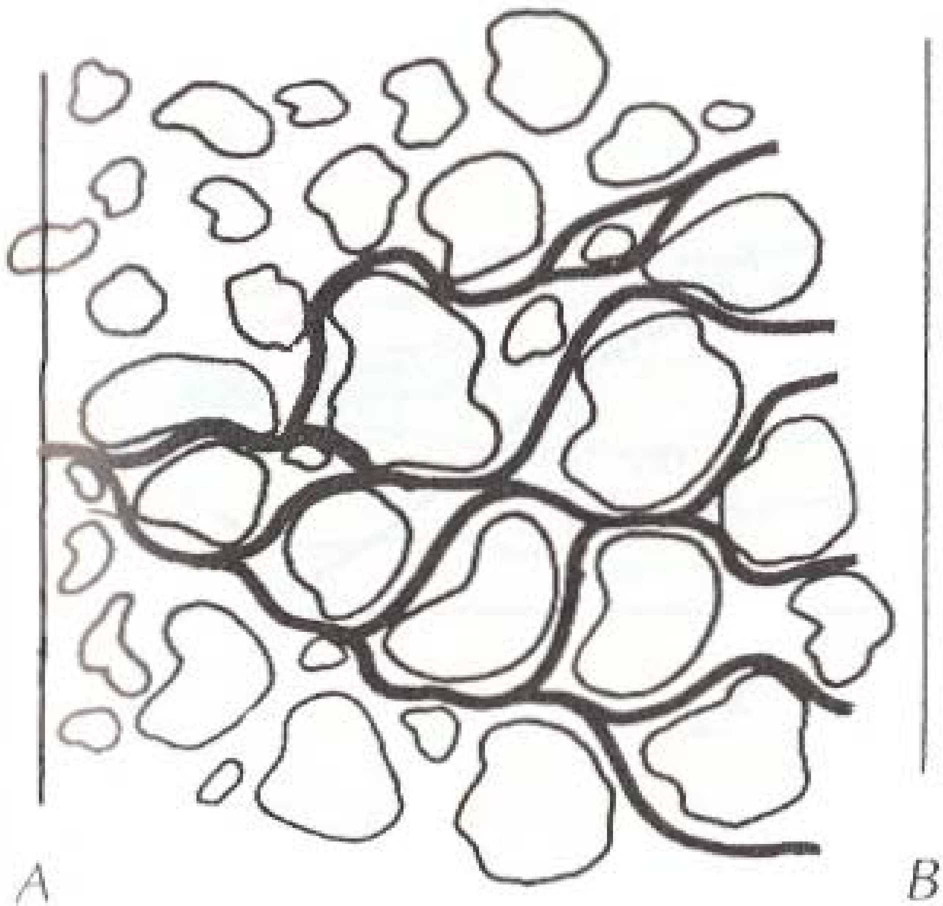
$$D_{M,L} = \alpha_L v_a$$

a_L = Longitudinal dispersivity [L]

v_a = Pore water velocity [L/T]

Variations in the flow field – point scale

Lateral dispersion



Lateral dispersion coefficient
(1D flow)

$$D_{M,T} = \alpha_T v_a$$

a_T = Lateral dispersivity

v_a = Pore water velocity

“Dispersion like” processes

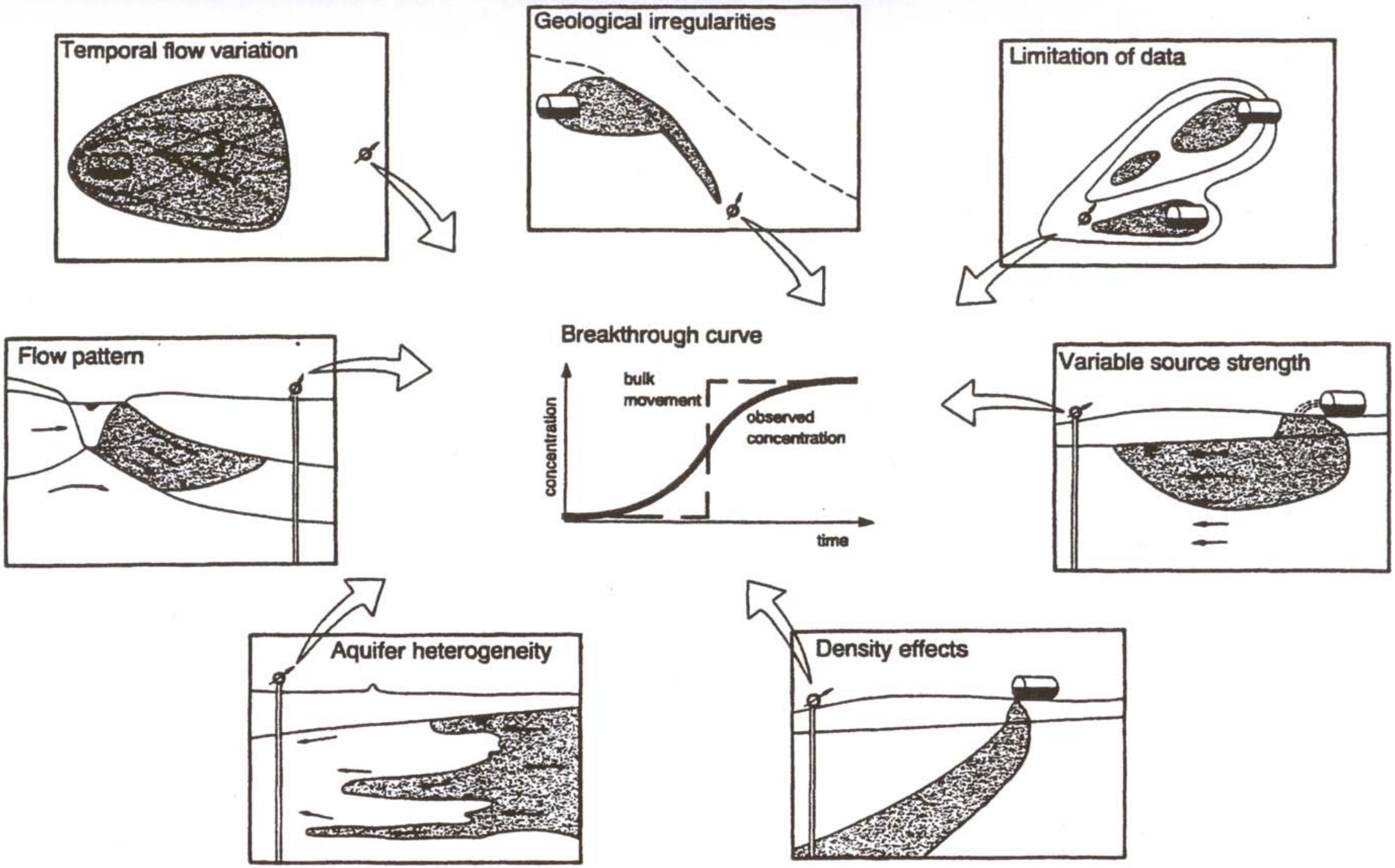
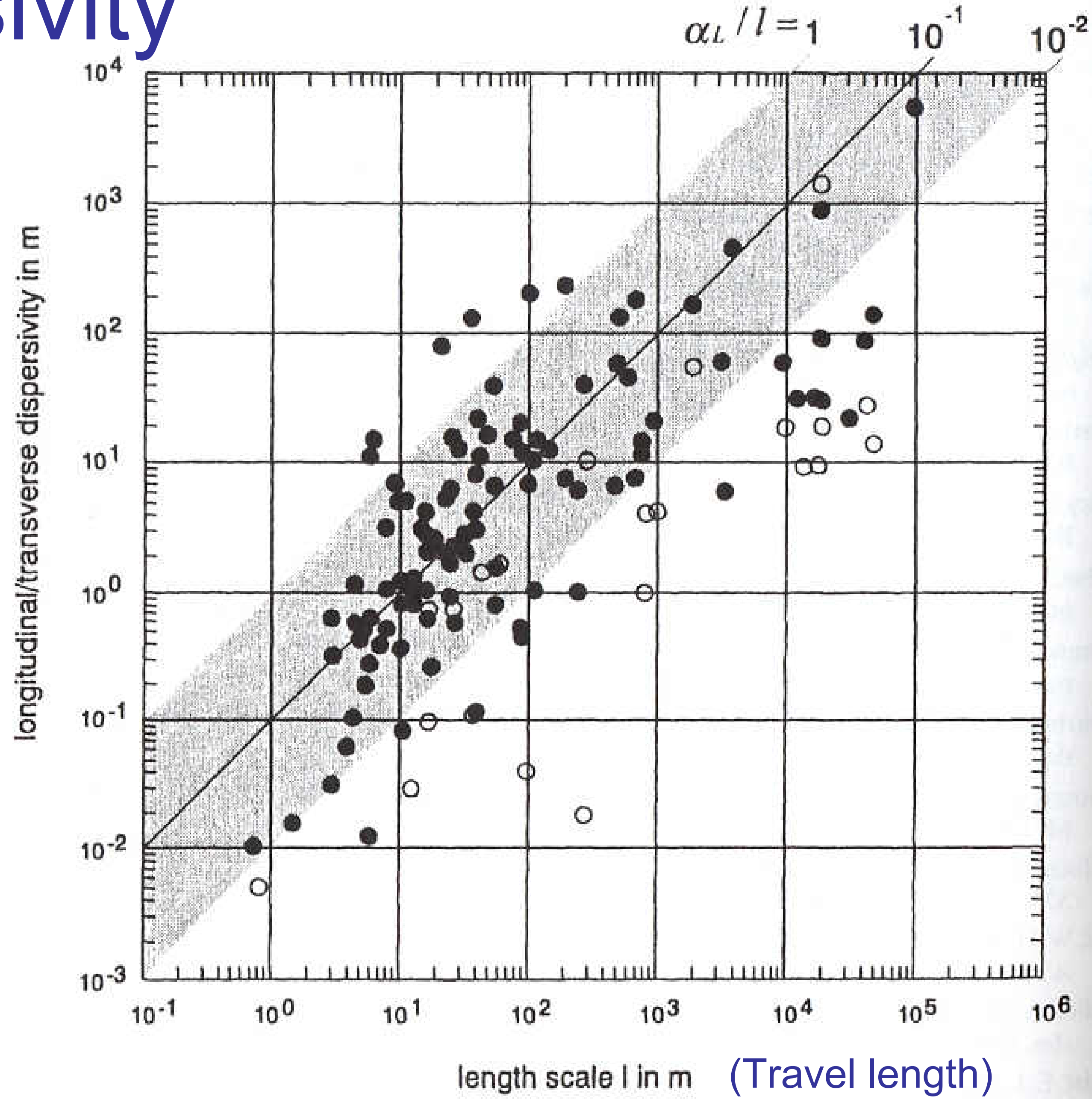


Figure 3.6 Factors which are likely to be interpreted as dispersion.

The dispersion processes are introduced because of incomplete description of advective flow …

→ scale dependent
→ “knowledge” dependent

Field dispersivity



(Travel length)

Dispersivity

$a_{i,j,k,l}$ = *4.order tensor*

Is often reduces to

a_L = longitudinal dispersivity

a_{TH} = lateral dispersivity in the horizontal plane

a_{TV} = lateral dispersivity in the vertical plane

or simply

a_L = longitudinal dispersivity

a_T = lateral dispersivity

Dispersion coefficients

Hydrodynamic dispersion coefficients (3D flow)

$$\mathrm{D}_{xx} = \alpha_L \frac{v_{a,x}^2}{|v_a|} + \alpha_{TH} \frac{v_{a,y}^2}{|v_a|} + \alpha_{TV} \frac{v_{a,z}^2}{|v_a|} + D^*$$

$$\mathrm{D}_{yy} = \alpha_L \frac{v_{a,y}^2}{|v_a|} + \alpha_{TH} \frac{v_{a,x}^2}{|v_a|} + \alpha_{TV} \frac{v_{a,z}^2}{|v_a|} + D^*$$

$$\mathrm{D}_{zz} = \alpha_L \frac{v_{a,z}^2}{|v_a|} + \alpha_{TV} \frac{v_{a,x}^2}{|v_a|} + \alpha_{TV} \frac{v_{a,y}^2}{|v_a|} + D^*$$

$$\mathrm{D}_{xy} = \mathrm{D}_{yx} = (\alpha_L - \alpha_{TH}) \frac{v_{a,x} v_{a,y}}{|v_a|}$$

$$\mathrm{D}_{xz} = \mathrm{D}_{zx} = (\alpha_L - \alpha_{TV}) \frac{v_{a,x} v_{a,z}}{|v_a|}$$

$$\mathrm{D}_{yz} = \mathrm{D}_{zy} = (\alpha_L - \alpha_{TV}) \frac{v_{a,y} v_{a,z}}{|v_a|}$$

D_{xx}, D_{yy}, D_{zz} = principle components in the dispersion tensor, L^2T^{-1}

$D_{xy}, D_{xz}, D_{yx}, D_{yz}, D_{zx}, D_{zy}$ = Cross components in the dispersion tensor, L^2T^{-1}

a_L = longitudinal dispersivity, L

a_{TH} = horizontal lateral dispersivity, L

a_{TV} = vertical lateral dispersivity, L

D^* = effective molecular diffusion coefficient, L^2T^{-1}

$v_{a,x}, v_{a,y}, v_{a,z}$ = components in the pore water velocity vector, LT^{-1}

$|v_a|$ = length of the velocity vector, LT^{-1}

Exercise

Spreading due to dispersion in a uniform stationary flow

The concentration plume that originates form a point injection follows a normal distribution with

$$\sigma_{\mathrm{L}} = \sqrt{2D_L t}$$

$$\sigma_{\mathrm{T}} = \sqrt{2D_T t}$$

A monitoring program is set-up 1000 m down stream

Calculate s_L and s_T at the monitoring station 1000 m down stream given:

$$\alpha_{\mathrm{L}} = 10\,\mathrm{m}$$

$$\alpha_{\mathrm{T}} = 1\,\mathrm{m}$$

$$v_{\mathrm{a}} = 0.1\,\mathrm{m/day}$$

What is s_L and s_T at the monitoring station if

$$v_{\mathrm{a}} = 0.5\,\mathrm{m/day}$$

Dispersion flux (1D flow)

Fick´s law

$$q_D = -D_L \frac{dC}{dx}$$

D_L = Longitudinal dispersion coefficient L^2T^{-1}

C = Solute concentration ML^{-3}

Dispersion and diffusion flux (1D strømning)

$$q_h = -D_h \frac{dC}{dx}$$

C = Solute concentration ML^{-3}

D_h = Longitudinal hydrodynamic dispersion coefficient L^2T^{-1}

$$D_h = D_L + D_0 = \alpha_L v_a + D_0$$

Total flux

Advection + dispersion (1D flow)

$$q_{\text{tot}} = qC - D_h \frac{dC}{dx}$$

q_{tot} = *Total flux* $MT^{-1}L^{-2}$

q = darcy velocity LT^{-1}

Total flux

advection + dispersion (3D flow)

$$\mathrm{q}_{\mathrm{tot,x}} = q_x C - D_{xx}\frac{dC}{dx} - D_{xy}\frac{dC}{dy} - D_{xz}\frac{dC}{dz}$$

Governing equation

1D advection-dispersion equation

$$\frac{\partial \theta C}{\partial t} = D_L \frac{\partial^2 \theta C}{\partial x^2} - \frac{\partial \theta v_a C}{\partial x} - S$$

D_L = longitudinal hydrodynamic dispersion coefficient, L^2T^{-1}

C = solute concentration, ML^{-3}

v_a = Pore water (transport) velocity LT^{-1}

S = sink/source due to sorption or decay, $ML^{-3}T^{-1}$

t = time, T

Governing equation

3D advection-dispersion equation

$$\frac{\partial \theta C}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial \theta v_{a,i} C}{\partial x_i} - S$$

D_L = components in the hydrodynamic dispersion tensor, L^2T^{-1}

C = solute concentration, ML^{-3}

v_a = components in the pore water velocity vector LT^{-1}

S = sink/source due to sorption or decay, $ML^{-3}T^{-1}$

R_n = chemical reactions, $ML^{-3}T^{-1}$

t = time, T

Sorption as a sink/source term, S_i

$$S_i = -\rho_b \frac{\partial C_a}{\partial t}$$

r$_b$ = bulk density, ML^{-3}

C_a = adsorbed concentration, MM^{-1}

$$\frac{\partial \theta C}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij} \frac{\partial C}{\partial x_j}\right) - \frac{\partial \theta v_{a,i} C}{\partial x_i} \boxed{- \rho_b \frac{\partial C_a}{\partial t}}$$

$$\Downarrow$$

$$\frac{\partial \theta C}{\partial t} + \boxed{\rho_b \frac{\partial C_a}{\partial t}} = \frac{\partial}{\partial x_i}\left(\theta D_{ij} \frac{\partial C}{\partial x_j}\right) - \frac{\partial \theta v_{a,i} C}{\partial x_i}$$

$$\Downarrow$$

$$\boxed{R \frac{\partial \theta C}{\partial t}} = \frac{\partial}{\partial x_i}\left(\theta D_{ij} \frac{\partial C}{\partial x_j}\right) - \frac{\partial \theta v_{a,i} C}{\partial x_i}$$

where $R = 1 + \frac{\rho_b}{\theta} \frac{\partial C_a}{\partial C}$ (Retardation factor)

Sorption

Equilibrium controlled sorption

Linear sorption

$$R = 1 + \frac{\rho_b}{\theta}\frac{\partial C_a}{\partial C} = 1 + \frac{\rho_b}{\theta} K_d$$

where

K_d = *distribution coefficient* $[L^3M^{-1}]$ $C_a = K_d\, C$

Numerical implementation

$$R\,\theta\,\frac{\partial C}{\partial t} = R_{i,j,k}\theta_{i,j,k}\,\frac{C_{i,j,k}^{n+1} - C_{i,j,k}^{n}}{\Delta t}$$

Sorption

Non-equilibrium controlled sorption

$$\frac{\partial \theta C}{\partial t} + \rho_b \frac{\partial C_a}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij} \frac{\partial C}{\partial x_j}\right) - \frac{\partial \theta v_{a,i} C}{\partial x_i}$$

$$\rho_b \frac{\partial C_a}{\partial t} = \beta\left(C - \frac{C_a}{K_d}\right)$$

b = First order mass transfer rate between dissolved and sorbed phases, T^{-1}

K_d = distribution coefficient for the sorbed phase

Numerical implementation

$$\rho_{b(i,j,k)} \frac{C^{n+1}_{a,i,j,k} - C^{n}_{a,i,j,k}}{\Delta t} = \beta_{i,j,k}\left(C^{n+1}_{i,j,k} - \frac{C^{n+1}_{a,i,j,k}}{K_{d(i,j,k)}}\right)$$

$$S_i = \beta_{i,j,k}\left(C^{n+1}_{i,j,k} - \frac{C^{n+1}_{a,i,j,k}}{K_{d(i,j,k)}}\right)$$

Decay/degradation

first order

$$S_i = \left(\lambda_1 \theta C + \lambda_2 \rho_b C_a\right)$$

Decay of dissolved solute

Decay of sorbed solute

l_1 = first order reactions rate for dissolved solute, T^{-1}

l_2 = first order reaction rate for sorbed solute, T^{-1}

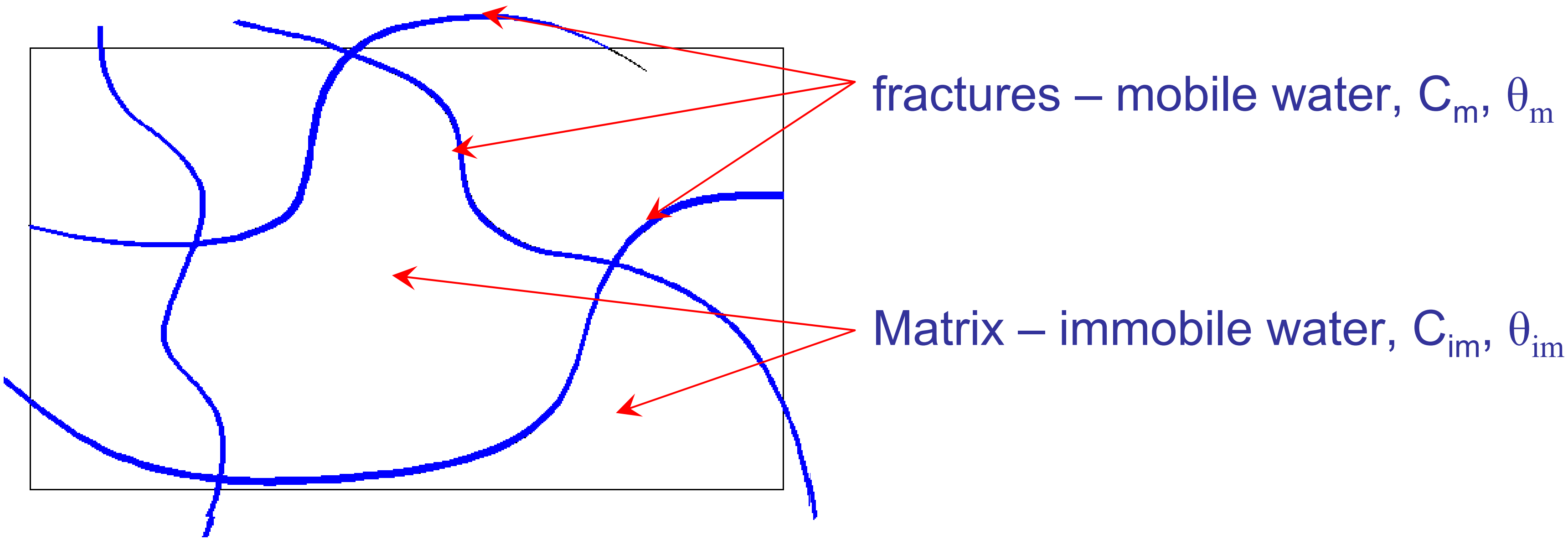
$$\lambda = \left(\ln 2\right) / t_{\frac{1}{2}}$$

$T_{½}$ = half life, T

Numerical implementation

$$S_i = -\lambda_1 \theta_{i,j,k} C^n_{i,j,k} - \lambda_2 \rho_{b(i,j,k)} C^n_{a,i,j,k}$$

Dual porosity systems



$$\frac{\partial \theta_m C_m}{\partial t} + \frac{\partial \theta_{im} C_{im}}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta_m D_{ij} \frac{\partial C_m}{\partial x_j}\right) - \frac{\partial \theta_m v_{a,i} C_m}{\partial x_i}$$

$$\frac{\partial \theta_{im} C_{im}}{\partial t} = \zeta \left(C_m - C_{im}\right)$$

ξ = Mass transfer rate between mobile and immobile water, T^{-1}

Dual porosity systems

$$\frac{\partial \theta_m C_m}{\partial t} + \frac{\partial \theta_{im} C_{im}}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta_m D_{ij} \frac{\partial C_m}{\partial x_j}\right) - \frac{\partial \theta_m v_{a,i} C_m}{\partial x_i}$$

$$\frac{\partial \theta_{im} C_{im}}{\partial t} = \zeta \left(C_m - C_{im}\right)$$

Numerical implementation

$$\theta_{im(i,j,k)} \frac{C^{n+1}_{im(i,j,k)} - C^{n}_{im(i,j,k)}}{\Delta t} = \zeta \left(C^{n+1}_{m(i,j,k)} - C^{n+1}_{im(i,j,k)}\right)$$

$$R_i = \zeta \left(C^{n+1}_{m(i,j,k)} - C^{n+1}_{im(i,j,k)}\right)$$

Solution of the 3D advection-dispersion equation

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - v_{a,i}\frac{\partial C}{\partial x_i} + S_n = \frac{\partial C}{\partial t}$$

- Standard finite difference methods
- Particle methods (random walk)
- Hybrid methods (MOC)
- High order FD or FV methods (TVD)